

# Diffusion in Curved Tube

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## Abstract

Particle diffusion in a curved tube embedded in  $R_3$  is considered. We find the diffusion coefficient depends on tube's curvature. Diffusion coefficient is obtained in  $\epsilon$  (radius of tube) expansion. Physical interpretation of curvature dependent diffusion coefficient is given.

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## I. INTRODUCTION

In the previous paper on surface diffusion with thickness embedded in  $R_3$  established the curvature dependence of surface diffusion [1]. This theory might be applied to the molecular diffusion in lipid bilayer or applied to the reaction diffusion system [2], [3].

However, the physical meaning of curvature dependence was not clear. To make clear this point we consider an one dimension less system, that is, the diffusion in tube embedded in  $R_3$ . The quantum mechanical version to this problem is given in [4], and higher dimensional extension is given in [5]. (This quantum mechanical problem was originally discussed by many authors [6], [7] to solve the ordering problem of quantum mechanics on curved space.) In the case of thin tube (string) in  $R_3$ , the dimensional difference is two and there appears additional degree of freedom to rotate around the central axis directions, so called torsion that makes calculation bit complicated. However the “local equilibrium condition” (explained later) makes the effect of torsion disappear, and we have the curvature dependent diffusion equation. The physical reason of its curvature dependence is discussed precisely in last section.

## II. FRENET-SERET EQUATIONS

Let us consider a line specified by

$$\vec{x}(s), \tag{1}$$

where the parameter  $s$  is the length of line. The unit tangent vector is defined by

$$\vec{e}_1 \equiv \frac{d\vec{x}(s)}{ds}. \tag{2}$$

Another (normal) unit vector  $\vec{e}_2$  is defined by equation.

$$\frac{d\vec{e}_1(s)}{ds} = \kappa \vec{e}_2, \quad |\vec{e}_2| = 1. \tag{3}$$

$\kappa$  is called the curvature of this line in  $R_3$ . The reason is the following. We can set a circle which tangents to this curved line at point  $\vec{x}(s)$ . From figure 1 we can easily find two relations.

$$\vec{e}_1(s + ds) - \vec{e}_1(s) = \vec{e}_2 d\theta, \tag{4}$$

$$ds = R d\theta, \tag{5}$$

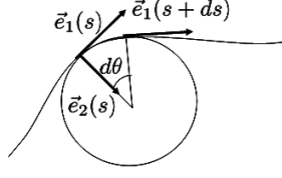


FIG. 1. Curvature

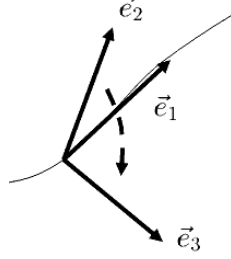


FIG. 2. Torsion

where  $R$  is the radius of this circle. Then we find the equation (3) with identifying  $\kappa = 1/R$ .

Next we introduce another independent unit vector  $\vec{e}_3$  by

$$\vec{e}_3 = \vec{e}_1 \times \vec{e}_2. \quad (6)$$

Then we can identify the derivation of  $\vec{e}_2$  generally such as,

$$\frac{d\vec{e}_2}{ds} = \alpha \vec{e}_1 + \tau \vec{e}_3, \quad (7)$$

where  $\alpha$  and  $\tau$  are unknown some functions. But  $\alpha$  can be calculated as follows.

$$\alpha = \vec{e}_1 \cdot \frac{d\vec{e}_2}{ds} = -\vec{e}_2 \cdot \frac{d\vec{e}_1}{ds} = -\kappa. \quad (8)$$

So we can replace (7) as

$$\frac{d\vec{e}_2}{ds} = -\kappa \vec{e}_1 + \tau \vec{e}_3. \quad (9)$$

Function  $\tau$  has a geometrical meaning.

From the equation

$$\tau = \frac{d\vec{e}_2}{ds} \cdot \vec{e}_3, \quad (10)$$

we see  $\tau$  means the rotation of normal vector  $\vec{e}_2$  around  $\vec{e}_1$  (figure 2). So this function is called torsion.

We further take a derivative of  $\vec{e}_3$ .

$$\frac{d\vec{e}_3}{ds} = \beta \vec{e}_1 + \gamma \vec{e}_2, \quad (11)$$

with unknown function  $\beta$  and  $\gamma$ . Both of them can be obtained as follows.

$$\beta = \frac{d\vec{e}_3}{ds} \cdot \vec{e}_1 = -\frac{d\vec{e}_1}{ds} \cdot \vec{e}_3 = -\kappa \vec{e}_2 \cdot \vec{e}_3 = 0. \quad (12)$$

and

$$\gamma = \frac{d\vec{e}_3}{ds} \cdot \vec{e}_2 = -\frac{d\vec{e}_2}{ds} \cdot \vec{e}_3 = -\tau. \quad (13)$$

So we obtain

$$\frac{d\vec{e}_3}{ds} = -\tau \vec{e}_2. \quad (14)$$

We call these three equations (3), (9), and (14) as Frenet-Serret equations, and we have two geometrical quantities, curvature  $\kappa$  and torsion  $\tau$ .

### III. METRIC IN TUBE

We re-identify the one dimensional diffusion on curved line as the limitation process from three dimensional diffusion. We set the curved tube with radius  $\epsilon$  in three dimensional Euclidean space  $R_3$ . Our particles can move only in this tube. We look for the form of diffusion equation in the limit of small  $\epsilon$ . The coordinates we use hereafter is the followings. (See FIG.3)

$\vec{X}$  is the Cartesian coordinate in  $R_3$ .  $\vec{x}$  is the Cartesian coordinate which specifies only the points on center line.  $q^i$  is the normal coordinate in a direction of  $\vec{e}_i$ . (Small Latin indices  $i, j, k, \dots$  runs from 2 to 3.)  $s$  is the length parameter along the center line. Further by using the normal unit vector  $\vec{e}_i$ , we can identify any points in tube by  $s, q^2, q^3$  by the following equation [4][5].

$$\vec{X}(s, q^2, q^3) = \vec{x}(s) + q^i \vec{e}_i(s), \quad (15)$$

where  $0 \leq |\vec{q}| \leq \epsilon$  with  $|\vec{q}| = \sqrt{(q^2)^2 + (q^3)^2}$ .

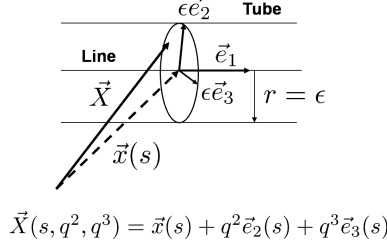


FIG. 3. Coordinate

From this relation we can obtain the curvilinear coordinate system in tube ( $\subset R_3$ ) by the coordinate  $q^\mu = (s, q^2, q^3)$ , and metric  $G_{\mu\nu}$ . (Hereafter Greek indices  $\mu, \nu, \dots$  runs from 1 to 3 with  $s = q^1$ .)

$$G_{\mu\nu} = \frac{\partial \vec{X}}{\partial q^\mu} \cdot \frac{\partial \vec{X}}{\partial q^\nu}. \quad (16)$$

Each part of  $G_{\mu\nu}$  is the following.

$$G_{11} = 1 - 2\kappa q^2 + (\kappa^2 + \tau^2)(q^2)^2 + \tau^2(q^3)^2, \quad (17)$$

$$G_{12} = -\tau q^3, \quad (18)$$

$$G_{13} = \tau q^2, \quad (19)$$

$$G_{23} = 0, \quad (20)$$

$$G_{22} = G_{33} = 1. \quad (21)$$

Compared to the previous paper, we have non zero off-diagonal elements. This comes from the fact that dimensional difference between outer space  $R_3$  and inner space  $R_1$  is two.

Now the following relations follow.

$$G \equiv \det(G_{\mu\nu}) = (1 - \kappa q^2)^2. \quad (22)$$

The inverse metric is given as,

$$G^{\mu\nu} = \frac{1}{(1 - \kappa q^2)^2} \times \begin{pmatrix} 1 & \tau q^3 & -\tau q^2 \\ \tau q^3 & (1 - \kappa q^2)^2 + (\tau q^3)^2 & -\tau^2 q^2 q^3 \\ -\tau q^2 & -\tau^2 q^2 q^3 & (1 - \kappa q^2)^2 + (\tau q^2)^2 \end{pmatrix}.$$

#### IV. DIFFUSION FIELD IN TUBE

Let us denote 3 dimensional diffusion field as  $\phi^{(3)}$ , and Laplacian as  $\Delta^{(3)}$ . Then we have the equation with normalization condition

$$\frac{\partial \phi^{(3)}}{\partial t} = D \Delta^{(3)} \phi^{(3)}, \quad (23)$$

$$1 = \int \phi^{(3)}(q^1, q^2, q^3) \sqrt{G} d^3 q, \quad (24)$$

where  $D$  is the diffusion constant, and  $G \equiv \det(G_{\mu\nu})$ . Our aim is to construct the effective one dimensional diffusion equation from 3D equation above.

$$\frac{\partial \phi^{(1)}}{\partial t} = D \Delta^{(eff)} \phi^{(1)}, \quad (25)$$

$$1 = \int \phi^{(1)}(s) ds, \quad (26)$$

where  $\phi^{(1)}$  is the one dimensional diffusion field, and  $\Delta^{(eff)}$  is unknown effective 1D diffusion operator which might not be equal to simple 1D Laplace Beltrami operator  $d^2/ds^2$ .

From two normalization conditions, we obtain

$$\begin{aligned} 1 &= \int \phi^{(3)}(q^1, q^2, q^3) \sqrt{G} d^3 q, \\ &= \int \left[ \int dq^2 dq^3 (\phi^{(3)} \sqrt{G}) \right] ds, \\ &= \int \phi^{(1)}(s) ds. \end{aligned}$$

Therefore we obtain the relation,

$$\phi^{(1)}(s) = \int \phi^{(3)} \sqrt{G} dq^2 dq^3. \quad (27)$$

We multiply  $\sqrt{G}$  to equation (23) and integrate by  $q^2, q^3$ , then we obtain

$$\frac{\partial \phi^{(1)}}{\partial t} = D \int (\sqrt{G} \Delta^{(3)}) \phi^{(3)} dq^2 dq^3. \quad (28)$$

From the form of Laplace Beltrami operator

$$\Delta^{(3)} = G^{-1/2} \frac{\partial}{\partial q^\mu} G^{1/2} G^{\mu\nu} \frac{\partial}{\partial q^\nu},$$

our diffusion equation has form

$$\frac{\partial \phi^{(1)}}{\partial t} = D \int \left( \frac{\partial}{\partial q^\mu} G^{1/2} G^{\mu\nu} \frac{\partial}{\partial q^\nu} \phi^{(3)} \right) dq^2 dq^3. \quad (29)$$

Here we suppose the “local equilibrium condition” such as,

$$\frac{\partial \phi^{(3)}}{\partial q^i} = 0, \quad i = 2, 3. \quad (30)$$

Because in direction of  $\vec{e}_2$ ,  $\vec{e}_3$ , equilibrium would be holds in a short time  $\delta t \sim \epsilon^2/D$ . When our observation is given in time scale  $t$  satisfying  $t \gg \delta t$ , we can always assume local equilibrium condition (30).

Then we have instead,

$$\begin{aligned} \frac{\partial \phi^{(1)}}{\partial t} &= D \int \left( \frac{\partial}{\partial q^\mu} G^{1/2} G^{\mu 1} \frac{\partial}{\partial s} \phi^{(3)} \right) dq^2 dq^3 \\ &= D \frac{\partial}{\partial s} \left( \int G^{1/2} G^{11} dq^2 dq^3 \right) \frac{\partial}{\partial s} \phi^{(3)} \\ &\quad + D \left\{ \int \frac{\partial}{\partial q^i} (G^{1/2} G^{i1}) dq^2 dq^3 \right\} \frac{\partial}{\partial s} \phi^{(3)}. \end{aligned} \quad (31)$$

From (27) and (30) we also have

$$\phi^{(3)} = \frac{\phi^{(1)}}{N}, \quad N = \int \sqrt{G} dq^2 dq^3 = \pi \epsilon^2. \quad (32)$$

So we obtain

$$\begin{aligned} \frac{\partial \phi^{(1)}}{\partial t} &= \frac{D}{\pi \epsilon^2} \frac{\partial}{\partial s} \left( \int G^{1/2} G^{11} dq^2 dq^3 \right) \frac{\partial}{\partial s} \phi^{(1)} \\ &\quad + \frac{D}{\pi \epsilon^2} \left\{ \int \frac{\partial}{\partial q^i} (G^{1/2} G^{i1}) dq^2 dq^3 \right\} \frac{\partial}{\partial s} \phi^{(1)}. \end{aligned} \quad (33)$$

The explicit calculation gives the integral.

$$\int \frac{\partial}{\partial q^i} (G^{1/2} G^{i1}) dq^2 dq^3 = 0, \quad (34)$$

and

$$\begin{aligned} \int G^{1/2} G^{11} dq^2 dq^3 &= \int \frac{dq^2 dq^3}{1 - \kappa q^2} \\ &= \pi \epsilon^2 \left\{ 1 + \left( \frac{\kappa \epsilon}{2} \right)^2 + \mathcal{O}(\epsilon^4) \right\}. \end{aligned} \quad (35)$$

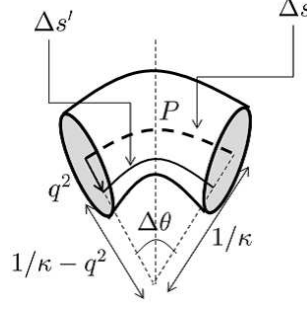


FIG. 4. Curved point

Then we come to the result.

$$\frac{\partial \phi^{(1)}}{\partial t} = \frac{\partial}{\partial s} D_{eff}(s) \frac{\partial}{\partial s} \phi^{(1)}, \quad (36)$$

with the definition of effective diffusion coefficient,

$$D_{eff} = D(1 + (\frac{\kappa \epsilon}{2})^2 + \mathcal{O}(\epsilon^4)). \quad (37)$$

The static solution has the form,

$$\phi^{(1)} = C_1 + C_2 \int_0^s \frac{ds'}{D_{eff}(s')}. \quad (38)$$

## V. PHYSICAL INTERPRETATION

We find the relation that,

$$D_{eff} = D < \frac{1}{1 - \kappa q^2} >, \quad (39)$$

where

$$< \dots > = \frac{1}{\pi \epsilon^2} \int dq^2 dq^3 \dots$$

Then we find the simple interpretation. Let us consider the point P on tube where the curvature is  $\kappa$ . We chose two sections near P, and discuss about the length connecting these two sections. See FIG.4. At the coordinate  $q^2$ , the length between two section is given by  $\Delta s' = (1 - \kappa q^2) \Delta s$ . Therefore the curvature dependence of effective diffusion coefficient is given by the mean value of rate of length i.e.,  $< \Delta s / \Delta s' >$ .

Next we consider the physical meaning. The diffusion coefficient is proportional to the mobility by Einstein's relation. The mobility is also proportional to the conductivity with



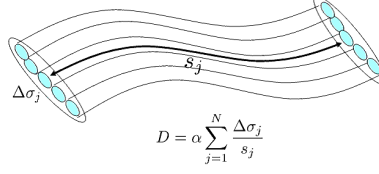


FIG. 5. Flux of Tubes

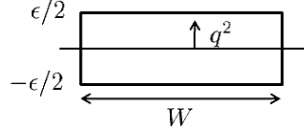


FIG. 6. another cross section

unit length and unit cross section. In the following we calculate the rate of conductivity between bent and straight for the same length and same cross section flux.

The conductivity of flux consist of  $N$  infinitesimal thin tubes is proportional to the sum of each conductivity of tubes. Each conductivity proportionals to the cross section  $\Delta\sigma_j$  and inversely proportionals to the length  $s_j$ . See FIG.5. So we have

$$D = \alpha \sum_{j=1}^N \frac{\Delta\sigma_j}{s_j}.$$

When the flux is straight with length  $\Delta s$ , each length is the same  $\Delta s = s_1 = s_2 = \dots$ , and so we obtain

$$D_{stra} = \alpha \sum_{j=1}^N \frac{\Delta\sigma_j}{s_j} = \frac{\alpha}{\Delta s} \left( \sum_{j=1}^N \Delta\sigma_j \right) = \frac{\alpha\sigma}{\Delta s},$$

where  $\sigma = \sum_j \Delta\sigma_j$ .

In the case of FIG.4, we have

$$D_{bent} = \alpha \sum_{j=1}^N \frac{\Delta\sigma_j}{s_j} = \alpha \int \frac{dq^1 dq^2}{(1/\kappa - q^2)\Delta\theta}.$$

(We consider the diffusion only in  $s$  direction since we used the local equilibrium condition.) So we obtain the rate

$$\frac{D_{bent}}{D_{stra}} = \frac{1}{\sigma} \int dq^1 dq^2 \frac{\Delta s}{(1/\kappa - q^2)\Delta\theta} = \frac{1}{\sigma} \int \frac{dq^1 dq^2}{1 - \kappa q^2}.$$

Then we obtain the result.

$$D_{bent} = \langle \frac{1}{1 - \kappa q^2} \rangle > D_{stra}.$$

On the other hand as we have shown as  $R = 0$  case in the previous paper [1], the curved surface with one direction has no curvature and other has finite curvature has anomalous diffusion coefficient such as,

$$D_{eff} \cong (1 + \epsilon^2 \kappa^2 / 12) D.$$

This relation also can be explained in this physical interpretation. In this case we consider the cross section as in FIG.6.

$$\begin{aligned} \langle \frac{1}{1 - \kappa q^2} \rangle &= \frac{1}{W\epsilon} \int_{-\epsilon/2}^{\epsilon/2} dq^2 \int_0^W dq^1 \frac{1}{1 - \kappa q^2} \\ &= \frac{1}{\epsilon} \int_{-\epsilon/2}^{\epsilon/2} dq^2 \{1 + \kappa q^2 + (\kappa q^2)^2 + \dots\} \\ &= 1 + \epsilon^2 \kappa^2 / 12 + \dots \end{aligned} \tag{40}$$

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